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Database of optical properties of cosmic dust analogues (DOP)

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Abstract. We present a database containing information on different aspects of calculation and usage of the optical properties of small *non-spherical* particles — cosmic dust analogues. The main parts of the DOP are a review of available methods of the light scattering theory, collection of light scattering codes, special computational tools, a graphic library of the optical properties (efficiencies, albedo, asymmetry factors, etc.), a database of the optical constants for astronomy, a bibliographic database of light scattering works, and links to related Internet resources. The general purpose of the DOP having the address *http://www.astro.spbu.ru/DOP* is twofold — to help scientists to apply the light scattering theory in astronomy and to give students and beginners a possibility quickly to get necessary knowledge on the subject.

Key words. databases, cosmic dust, light scattering

1. Introduction

Dust has been detected in most astronomical objects — from the Solar system to active galactic nuclei, and everywhere the dust grains were found to play an important role in different physical and chemical processes. Modelling of these objects should include accurate consideration of scattering, absorption and emission of radiation by the dust grains.

So far in such a modelling one mainly utilized the model of homogeneous spherical particles, though there are many evidences that the interstellar grains are mostly non-spherical and inhomogeneous. Today enough possibilities exist to avoid the use of the spherical model. To help scientists to make this step, we have developed a database including useful information, data, codes, references and links and made it accessible via the Internet. As far as we know there are no analogous databases in the World Wide Web.

In this paper our database having the address *http://www.astro.spbu.ru/DOP* is described first briefly, and then partly in more detail. The database contains various introductory notes written for students and beginners and more specific information on light scattering theory and its applications. The DOP includes many pieces of the review "Optics of cosmic dust" by Voshchinnikov (2002) and materials being used in lectures on physics of interstellar matter in the St. Petersburg University.

2. General overview of the database

The information, resources, and links presented in the DOP are collected in three main blocks:

1) those related with the theoretical aspects — scatterer models, methods of their realization, bibliography;

2) those connected with calculations (and hence applications) — optical constants, light scattering codes, graphic and tabular libraries of the optical properties, special tools;

3) those coupled with other topics (e.g., radiative transfer modelling).

The database has the following sections and subsections:

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A. **Theoretical aspects**
  A1. Definitions of the optical characteristics of non-spherical scatterers
  A2. Scatterer models and their parameters
  A3. Exact and approximate methods of light scattering theory
  A4. Light scattering experiments
  A5. Bibliography of light scattering works

B. **Application aspects**
  B1. Optical constants of materials
  B2. Light scattering codes
  B3. Benchmark results
  B4. A graphic library of the optical properties
  B5. Self-training algorithm for calculation of the optical properties of fractal-like aggregates

C. **Related resources**
  C1. Radiative transfer tools
  C2. Miscellaneous

Let us now turn to a brief description of the subsections.

2.1. DOP subsections on theoretical aspects (part A)

Here we first define the cross-sections, albedo, scattering matrix and other *basic optical characteristics of non-spherical scatterers* and compare them with those for spherical particles. The idea is to supplement and compress information given in other sources of such definitions (see Mishchenko et al., 2000, 2002)

The *parameters of non-spherical scatterers* (size, shape, etc.) are briefly discussed in the next subsection and the light scattering models popular in astronomy (spheres, cylinders, spheroids, aggregates) are listed in there.

To realize any scattering model, i.e. to obtain its optical properties, one should select a proper exact or approximate light scattering method. We make an *overview of various light scattering methods* and cite several other useful reviews of this kind. A special very detailed review of the methods was prepared by N.G. Khlebtsov (see Sect. 3.1 for more details)

The optical properties of cosmic dust analogues can be also measured in laboratory. References to two available WWW *databases of such measurements* are presented.

The last subsection is devoted to *bibliography on light scattering theory and its various applications* which is considered in detail in the Sect. 3.2.

2.2. DOP subsections on application aspects (part B)

Here we start with definitions of *optical constants (refractive indices or dielectric functions) of materials* and link the Jena-St. Petersburg Database of Optical Constants for astronomy (JPDOC) developed earlier. This database described by Henning et al. (1999) and Jäger et al. (2003) consists of original laboratory data, references and links to resources related to measurements and calculations of the optical constants for materials important for astronomical applications. More information on this part is presented in Sect. 3.3.

The next subsection contains a set of *light scattering codes* developed by us and used in astronomical applications. Links to other collections of such codes are also given.

To test a code not used before one often needs some well checked results. The optical characteristics of spheroidal particles of different size, shape, and refractive index calculated by several methods are given in our *benchmark* subsection.

An important part of the database is the *graphic library of the optical properties* of different scatterer models — homogeneous and core-mantle spheres, homogeneous and core-mantle cylinders, homogeneous spheroids. In another part of this subsection the properties of dust grains which can be estimated from the observations of the interstellar extinction and polarization are discussed (see Sect. 3.4 for more details).

The DOP also includes description and computer realization of a *self-training algorithm to predict the optical properties* of fractal-like aggregates. As this tool was not yet properly outlined in the literature, Sect. 3.5 is devoted to its brief description.

2.3. DOP subsections with related resources (part C)

The optical properties are very often used in *radiative transfer* (RT) calculations. Therefore, we concern this point as well as list the RT methods and the majority of the RT codes used in astronomy.

The last subsection contains links to different *related resources* (like other databases of light scattering codes, electronic newsletters, etc.) which might be of some use in the DOP context.

3. A more detailed description of some parts of the database

3.1. Review of light scattering methods for non-spherical particles (A3)

The review consists of two parts — an bibliographic overview of history and development of several basic methods and a comparison of all available approaches to solution of the light scattering problem for non-spherical particles.

The overview made by N.G. Khlebtsov concerns both the exact (separation of variables, point matching, integral equations, coupled dipoles, T-matrix) and approximate [Rayleigh, Rayleigh–Gans–Debye (RGD) and its generalizations, anomalous diffraction, eikonal, geometrical optics (GO), perturbation, etc.] methods. In this review the history of development of the methods is traced in very careful manner. The works on the applicability range and various applications of the methods are referred as well, and all together there are over 500 cited papers.

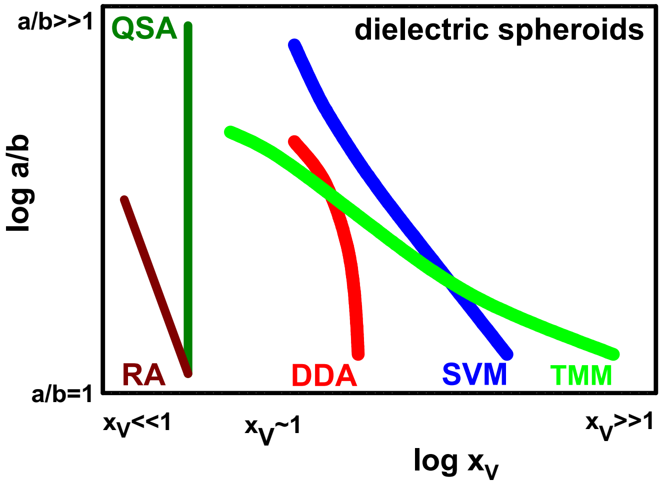

Fig. 1. Applicability ranges (domains left to the curves) of different methods in the case of dielectric prolate spheroids (a/b is the semiaxis ratio, x_V the size parameter of equivolume sphere). Calculations were made with codes based on the Rayleigh (RA) and quasistatic (QSA) approximations, the discrete dipole (DDA), separation of variables (SVM) and T-matrix (TMM) methods.

The comparison of methods is made in form of a table for 11 main approaches:
— separation of variables method,
— discretized Mie formalism,
— finite element method,
— finite difference method,
— point matching method,
— generalized multipole technique,
— extended boundary conditions method,
— method of moments,
— coupled dipoles method,
— Fredholm integral equation method,
— ray tracing/Monte Carlo method.

These approaches are classified and their ability to treat particles of different shape and structure as well as anisotropic and chiral scatterers and ensembles of particles is considered. For each method, references to the ansatz and some recent reviews are given. Comments to the table show the relationships and differences of the approaches, briefly concern their classifications and features, sources of available codes, and refer to works on comparison of the methods and other reviews.

We have also started the numerical investigation of applicability ranges of most popular methods using the spheroidal model of scatterers. An example of the results is given in Fig. 1 (see Il'in et al., 2002 for more details).

3.2. Bibliography on light scattering and its applications (A5)

Besides the review, the DOP also includes a special searchable bibliographic database on light scattering theory and its various applications. This bibliography being collected for over 15 years by V.A. Babenko consists of the following parts:
— *spherical homogeneous particles* — methodological questions, functions, calculations, internal fields, resonances, near field, etc.
— *inhomogeneous spheres* — layered, with radial and chaotic internal inhomogeneities, with inclusions, resonances, etc.
— *approximations for homogeneous spheres* — GO, Rayleigh, RGD, eikonal, van de Hulst (anomalous diffraction), and so on approximations;
— *complicated problems* — beam scattering, scattering by charged spheres, by rough, anisotropic and chiral particles, etc.;
— *cylindrical particles* (see below);
— *non-spherical objects* — works on different approaches and methods;
— *specific scattering media* — interstellar particles, marine particles, metallic zoles, powders, etc.;
— *carbon*;
— *ice*;
— *water*;
— *agglomerates, fractals*;
— *non-linear and mechanical effects in aerosols*;
— *vaporization and explosion of particles*;
— *inverse problems*;
— *laboratory experiments*;
— *laser remote sensing*;
— *radiative transfer*;
— etc.

To demonstrate the wideness of the questions considered we shall exemplify a full list of subsections for the section on cylindrical particles:
— circular infinite cylinders;
— oblique incidence and orientation averaging;
— multi-layered cylinders;
— GO approximation (including hexagonal cylinders);
— cylinders with smooth radial inhomogeneity;
— gyrotropic, gyroelectric and anisotropic cylinders;
— internal and near fields;
— experiments on cylinders;
— morphological resonances;
— van de Hulst approximation for cylinders;
— Rayleigh and RGD approximations;
— Hart-Montroll and S-approximations;
— non-circular infinite cylinders;
— circular cylinder of finite length and discs.

The total number of included references exceeds 8000 and each subsection contains several dozens of references.

3.3. Optical constants for cosmic dust analogues (B1)

This part of the DOP includes some notes introducing the optical constants required by astronomy, and links the optical constants database (JPDOC). The JPDOC consists of two main parts. One is the bibliography on optical con-

Table 1. Jena data currently available from the JPDOC

Compound	Composition	State	Low temperature measurements	Spectral regions
silicates	(Mg,Fe)SiO_3, $(Mg,Fe)_2SiO_4$	glassy	yes	ultraviolet – infrared
	$MgSiO_3$, $(Mg,Fe)_2SiO_4$	crystalline	yes	infrared
	$MgSi_xO_y$	amorphous	yes	ultraviolet – infrared
	(Ca,Al,Mg,Fe)Si_xO_y	amorphous	no	infrared
sulfides	(Mg,Fe)S	crystalline	yes	infrared
	SiS_2	crystalline	no	infrared
oxides	(Mg,Fe)O	crystalline	yes	ultraviolet – infrared
	Al_2O_3	amorphous	no	infrared
	$(Mg,Al)O_x$	crystalline	no	infrared
carbon	a-C:H	amorphous	no	ultraviolet – infrared

stants of astronomically interesting materials:
— amorphous/glassy/crystalline silicates of different kinds;
— silicon, SiO, crystalline/fused SiO_2;
— metals: Fe, Mg, and others;
— oxides: FeO, Fe_2O_3, Fe_3O_4, MgO, Al_2O_3, $MgAl_2O_4$;
— sulfides: FeS, MgS, SiS_2;
— carbides: SiC, FeC, TiC;
— carbonaceous species: diamonds, graphite, coals, kerogens, HAC, glassy/amorphous carbon, PAHs and so on;
— organics: tholin, "organic refractory", etc.
— ices: H_2O, CO, CO_2, NH_3, HCN, etc. and their mixtures;
— FeSi, $CaCO_3$ and some other materials.
We tried to include all papers published since the beginning of the previous century (all together over 700 references).

Another part is a set of data specially measured in the Jena laboratory for astronomical purposes. Note that although various terrestrial analogues of cosmic solids have been studied in chemical and physical laboratories, many of these experiments neither took into account the specifics of cosmic dust materials (composition, lattice structure, etc.) and conditions (low temperature, processing, etc.), nor covered the wavelength intervals of the current astrophysical interest.

A summary of the data obtained in Jena and made available is given in Table 1; data examples are presented in Fig. 2 (see Jäger et al., 2003 for more examples).

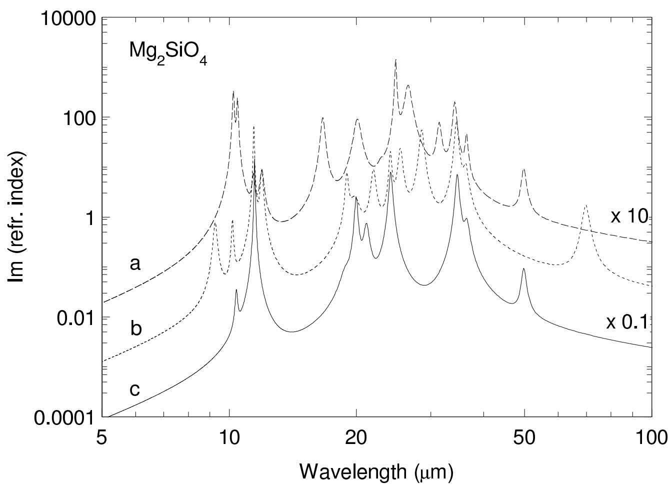

Fig. 2. Imaginary part of the refractive index for crystalline forsterite (Mg_2SiO_4) in the three different crystallographic directions.

3.4. Graphic library of optical properties of non-spherical scatterers (B4)

This DOP section consists of two parts — a basic graphic library and special notes on optical properties of cosmic dust analogues and their connection with observed manifestations of interstellar dust.

In the basic library we show how different optical characteristics (extinction, scattering and absorption efficiencies, albedo, asymmetry factor, etc.) vary with scatterer parameters: the real (n) and imaginary (k) parts of the refractive index, size (the refractive index is kept independent of radiation wavelength), shape, structure. So far we have considered homogeneous and core-mantle spheres and infinite cylinders, and homogeneous spheroids, but are planning to involve more scatterer models. The figures in the DOP are given for weakly absorbing ($n = 1.3 - 1.7$, $k = 0 - 0.3$) and highly absorbing ($n = 1.5 - 3.5$, $k = 0.5 - 2.5$) particles (see Fig. 3 for examples). These refractive indices are typical of astronomically interesting materials in visual.

The special notes are the chapters of the review of Voshchinnikov (2002) which cover the following questions of observed phenomena modelling — extinction efficiencies: general behaviour and deviations, wavelength dependence, the 2175 A feature, absolute extinction and abundances, etc.; polarization efficiencies: size/shape/orientation effects, linear polarization: wavelength dependence, circular polarization: change of sign and so on. Some more chapters will be included in the near future.

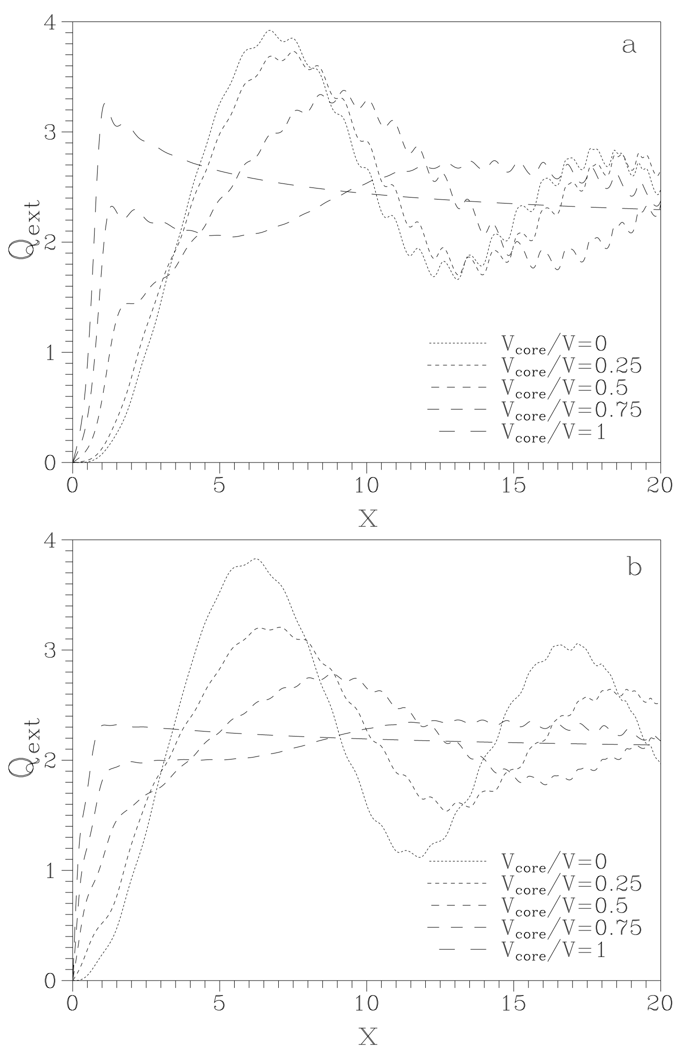

Fig. 3. The extinction factors for core-mantle spheres (a) and infinite cylinders (b) of different core size (volume).

3.5. *Self-training algorithm for fractal-like aggregates (B5)*

This part of the DOP was developed in Kharkov University by V.P. Tishkovets, S.A. Beletsky and P.V. Litvinov. Its idea is as follows — as calculations of the optical properties of subparticle aggregates need a huge amount of processor time, it is worthwhile to construct a self-training algorithm that could learn to predict the properties analyzing a limited set of these data.

To reduce the number of free parameters, fractal-like aggregates of equal size subparticles were selected. The structure of the aggregates can be characterized by two parameters: the fractal dimension D and the prefactor constant ρ (see, e.g., Feder, 1988). Other parameters are the number of subparticles N, the size parameter x and the real and imaginary parts of the refractive index of subparticles.

The algorithm was based on an artificial neural network named 'multi-layered perceptron' (see, e.g., Miller, 1990 for more details). A model of perceptron with 6 input and 30 output neurons and two layers with 30 neuron in each between the input and output ones was used. The algorithm was realized in the form of Pascal and Fortran codes. The region of its training was $n = 1.4-1.7$; $k = 0.001 - 0.1$; $x = 1.5$; $D = 3$; $\rho = 8$; $N \leq 50$. Accurate calculations were done by the Mackowski and Mishchenko (1996) code. The results were the expansion coefficients of the scattering matrix elements in series of the generalized spherical functions for particles of different N, refractive index, etc. Figure 4 shows the accuracy of the perceptron results.

The codes and data archive as well as documentation are available via the DOP. Our work with the perceptron on modelling of the optical properties of interplanetary dust grains has demonstrated its advantages due to extremely small size of the codes and very fast data access.

4. Concluding remarks

We have introduced a database of the optical properties of cosmic dust analogues. It is designed for student and scientists to help in applications of non-spherical scatterer models in astronomy but can be useful in other scientific fields as well.

A further development of the database is planed in near future. It will include a graphics interface for the JPDOC, a special tool for on-line calculations of different optical properties of non-spherical layered particles, more chapters from Voshchinnikov's (2002) review and its continuation, and so on.

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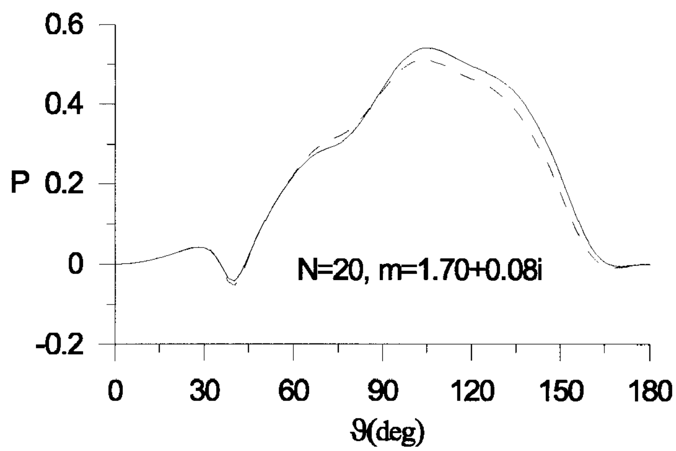

Fig. 4. Linear polarization degree P versus the scattering angle θ. Solid curve corresponds to the accurate values, dotted one to values given by the perceptron. The number of subparticles in an aggregate $N = 20$, $m = 1.7 + 0.08i$.

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